Climate change and global warming

Tuckett, Richard

DOI:
10.4172/2161-0398-C3-033

Document Version
Publisher's PDF, also known as Version of record

Citation for published version (Harvard):
Tuckett, R 2018, 'Climate change and global warming: thoughts of a Quaker scientist', *Journal of Physical Chemistry and Biophysics*, vol. 8, no. 4, Supplement, pp. 62-63. https://doi.org/10.4172/2161-0398-C3-033

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Keynote Forum

Day 1

Horst Köppel, J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-033

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Horst Köppel

University of Heidelberg, Germany

Non adiabatic molecular dynamics following photoexcitation: an *ab initio* quantum approach

The author will present an overview over the theoretical work on molecular dynamics following photoexcitation in the visible or UV spectral range. This carries the system to an electronically excited state with a potential energy surface (PES) differing from that of the electronic ground state. A rich variety of vibrational and related processes will thus be initiated which can proceed on a single or several of the many different excited-state PESs. If some of these PESs are close in energy they interact and the nuclear motion on them does not proceed independently. This is the realm of nonadiabatic molecular dynamics which has been in the focus of interest of spectroscopists and physical and theoretical chemists for many years. It is of fundamental importance for many different excited-state processes in biology, chemistry and physics (such as charge transfer, photochemical rearrangements etc.). A typical scenario are so-called conical intersections of potential energy surfaces where different PES become degenerate upon variation of two nuclear coordinates. Systems treated by us recently comprise SO_2, small polyenes like butadiene or hexatriene or the benzene cation. Key features of the systems and methods used will be highlighted in the talk.

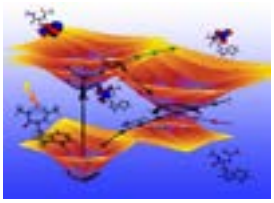


Figure 1: Schematic representation of two conical inter-sections and their associated photochemical reaction pathways.

Recent Publications

1. Teller E (1941) The crossing of potential surfaces. Journal of Physical Chemistry. 41(1):109-116.
2. H Köppel, W Domcke and L S Cederbaum (1984) Multimode Molecular dynamics Beyond the Born-Oppenheimer approximation. In Advances in Chemical Physics. 57:59-246.
3. W Domcke, D R Yarkony and H Köppel, Eds. (2011) Conical Intersections: Theory, Computation and Experiment. In Advanced Series in Physical Chemistry. World Scientific. Pages:768. Doi:10.1142/7803.
4. C Lévêque et al. (2013) *Ab initio* quantum study of the photodynamics and absorption spectrum of SO_2. The Journal of Chemical Physics. 138(4): 044320.
5. A Komainda et al. 2016) *Ab initio* benchmark study of nonadiabatic S1-S2 photodynamics of cis-and trans-hexatriene. The Journal of Physical Chemistry A. 120(33):6541-6556.

Biography

Horst Köppel has been a Senior Lecturer, and later Professor of Theoretical Chemistry at Heidelberg University since 1991. His research interests focuses on the theory of the Jahn-Teller effect, molecular excited state processes and vibrational structure in electronic spectra; special focus is on phenomena which cannot be described within the conventional Born-Oppenheimer separation of electronic and nuclear motions. He has authored and coauthored about 250 peer-reviewed original research papers, edited three books with topical reviews and organized several conferences in the field.

horst.koeppel@pci.uni-heidelberg.de

Pavel Hobza, J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-033

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Pavel Hobza

Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic

Noncovalent interactions in bio- and nanosciences: quantum mechanical aproach

Noncovalent interactions play an important role in chemistry, physics and biology. Reliable characteristics like stabilization energy, structure and vibrational frequencies are obtained using composite coupled cluster schemes which offer the possibility of improving the accuracy of results obtained by adding excitation operators of increasing order. It was shown that already CCSD(T)/CBS method yields an accurate and reliable description of noncovalent interactions, yet is only applicable to systems with several tens of atoms. Lower-level methods like DFT or semiempieical QM (SQM) should be parametriezed or verified and here the databases of accurate stabilization energies and geometries developed in our laboratory (S22, S66, X40 and L7) play an indispensable role. Binding free energy for host-guest and protein-ligand complexes is constructed as a sum of gas-phase interaction energy (ΔEint), change of desolvation free-energy (ΔΔGsolv), change of the conformational free energy of both components (ΔGconfw) and entropy term (eq. 1): $\Delta G_w \approx \Delta E_{int} + \Delta\Delta G_{solv} + \Delta G_{confw} - T\Delta S$ (1). Because of the size of systems investigated the DFT-D, and PM6 or SCC-DF-TB SQM methods combined with COSMO technique were considered. Performance of these methods was verified by comparison of interaction energies of model complexes with the benchmark values obtained from CCSD(T) and MP2.5 methods. Applicability of procedures described is demonstrated for evaluation of binding free energies of several extended systems like host – guest, protein – ligand and surface – admolecule ones.

Recent Publications

1. Rezac J and Hobza P (2016) Benchmark calculations of interaction energies in noncovalent complexes and their applications. Chem. Rev. 116(19):5038-5071.
2. Hostas J et al. (2016) A nexus between theory and experiment: non-empirical quantum mechanical computational methodology applied to cucurbit[n]uril.guest binding interactions. Chem. Eur. J. 22(48):17226-17238.
3. Sigwalt D et al. (2017) Unraveling the structure-affinity relationship between Cucurbit [n]urils (n=7, 8) and cationic diamondoids. J. Am. Chem. Soc.139():3249-3258.
4. Pecina A et al. (2017) QM/COSMO Scoring function at the DFTB3-D3H4 level: unique identification of native protein-ligand poses J. Chem. Inf. Model. 57:127-132.

Biography

Pavel Hobza (dr.hc, FRSC) obtained his PhD (1974) from the Institute of Physical Chemistry of the Academy of Science of the Czech Republic. He is a Distinguished Chair at the Institute of Organic Chemistry and Biochemistry of the Academy of Sciences of the Czech Republic, Prague, Czech Republic. His research team works on noncovalent interactions and their applications in bio- and material sciences, databases of accurate interaction energies and on *in silico* drug design. He has co-authored 4 books, more than 450 papers and 35 review papers in peer-reviewed journals, his H-index (WOS) is 98, sum of Times Cited is more than 35,000. He was awarded by "Highly Cited Researcher" in chemistry during 2014-2016 (Thomson Reuters, later Clarivate Analytics) and Schrödinger Medal in 2017 (World Association of Theoretical and Computational Chemists).

pavel.hobza@uochb.cas.cz

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Keynote Forum

Day 2

Richard Tuckett, J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-033

5th International Conference on

Physical and Theoretical Chemistry

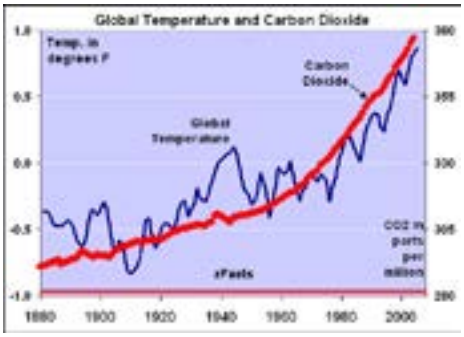
October 11- 13, 2018 | Edinburgh, Scotland

Richard Tuckett

University of Birmingham, UK

Climate change and global warming: thoughts of a Quaker scientist

This talk arises from two articles recently accepted for publication by Elsevier in their Reference Modules [1,2]; the first also comes out next year in paper copy in the 3rd edition of Encyclopaedia Analytical Sciences, Written for the intelligent non-expert, the science of the greenhouse effect and the most up-to-date data are presented in the first article [1]. In summary, the two most significant secondary greenhouse gases remain CO_2 and CH_4, together they contribute c. 80-85% of the secondary greenhouse effect, and this percentage has not changed for the last 20-30 years. CH_4 could indeed prove to be as serious a secondary greenhouse gas as CO_2. However, the total radiative forcing which causes the increase in Planet Earth's temperature has increased consistently over this time window, and the huge majority of the world's scientists now accept that we have a huge environmental issue on our hands that will not disappear. In the second article [2], suggestions are made as what issues people should think about from individual, government and world positions. The author is a practicing member of the Quaker (Society of Friends) religion, and throughout he comes to this problem from a moral viewpoint. This will not be a talk about religion, but rather how the six Quaker Testimonies (i.e. way we should lead our lives) on Truth and Integrity, Social Justice, Equality, Simplicity, Peace and Sustainability lead him in certain personal directions, and what advice he might give to Governments and World organisations (e.g. the United Nations). A concise and simple explanation of the Quaker religion in the UK in 2017 is written elsewhere [3]; much of it may surprise many delegates!.



The average temperature of the Earth (red) and the concentration level of CO_2 in the Earth's atmosphere (in red) during the recent history since AD1880. (Stoft http://zfacts.com/p/226.html or Hocker http://wattsupwiththat.com/2010/06/09/). A rise of 1 F is equivalent to 0.56°C. From a scientific viewpoint, there is no proven correlation between the two sets of data

Recent Publications:

1. Tuckett R P (2018) Greenhouse Gases Reference Module *Chemistry, Molecular Sciences and Chemical Engineering* (Elsevier, ScienceDirect). https://doi.org/10.1016/B978-0-12-409547-2.14031-4 . Also in *Encyclo. Analyt, Sciences* (2019) 3rd ed.
2. Tuckett R P (2018) Climate Change / Global Warming : what can we do, what should we do? Reference Module *Earth Systems Environmental Sciences* (Elsevier, ScienceDirect). DOI not yet published.
3. Rowlands H (ed.) 2017 God, words and us. Quaker Friends House, ISBN: 978-1-9997269-2-8.

Biography

Richard Tuckett completed his PhD in near-infrared spectroscopy in 1979. He first worked in electronic fluorescence spectroscopy of free radicals and molecular cations, often using supersonic beams and non-resonant electron excitation. From the late 1980s, he started using tunable vacuum-ultraviolet photon excitation from a synchrotron as a resonant ionisation source. In recent years he has studied the ionisation properties of long-lived greenhouse gases by threshold photoelectron and photoelectron photo-ion coincidence spectroscopy. Almost by accident, this has led him into atmospheric sciences and a wide interest in climate issues.

r.p.tuckett@bham.ac.uk

Notes:

Alexander Lorenz, J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-033

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Alexander Lorenz

Paderborn University, Germany

University of Kassel, Germany

Manipulating liquid crystals via photo generated fields and tailored polymer

Liquid crystals (LCs) are well-known for their highly sensitive and tuneable optical properties. However, inorganic-organic hybrids with localized, light induced (opto-optical) responses and LC composites with fast or threshold-free switching are sought after. In addition to conventional modulation of the intensity, the main goal is to tune optical phase shifts of incident light waves. Localized optical responses can be triggered by the use of light, to allow for optical manipulation. Photo generated polymer can yield in highly responsive, fast LC composites for future displays and adaptive optics.

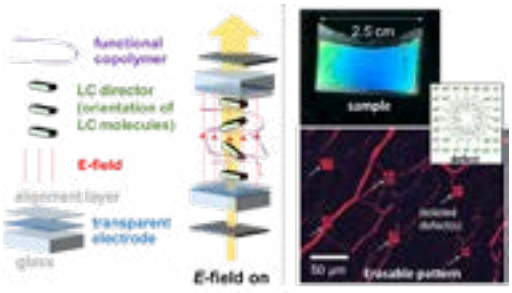


Figure 1: Schematic of a polymer network LC sample and polarized optical micrographs of a hybridized sample with photoinduced, erasable defect pattern.

Recent Publications:

1. Habibpourmoghadam A et al. (2017) Laser-induced erasable patterns in a N* liquid crystal on an iron doped lithium niobate surface. Optics Express 25(21):26148-26159.
2. Habibpourmoghadam A et al. (2017) Optical manipulation and defect creation in a liquid crystal on a photo responsive surface. Physical Review E 96(2-1):022701. Doi:10.1103/PhysRevE.96.022701.
3. Lorenz A et al. (2017) Nematic copolymer network LCs for swift continuous phase modulation and opaque scattering states. Mol. Cryst. and Liq. Cryst. 646(1):220-225. Doi:10.1080/15421406.2017.1288001.
4. Lorenz A, Braun L and Kolosova V (2016) Continuous optical phase modulation in a copolymer network nematic liquid crystal. ACS Photonics 3(7):1188-1193. Doi:10.1021/acsphotonics.6b0072.

Biography

Alexander Lorenz graduated from the Centre of Optoelectronics and Photonics Paderborn (Germany) in 2010 and has since conducted research at other leading institutions. He is the research Group Leader in the Department of Chemistry at the Paderborn University, Germany. His present research interests are photo generated polymer-liquid crystal hybrids and inorganic-organic liquid crystal hybrids with high responsiveness and fast performance. He has completed Deutsche Forschungsgemeinschaft (DFG)- (a German research funding organization) -Research Fellowships in the Department of Engineering of the University of Cambridge UK and TU Berlin; led research projects funded by TU Berlin, DFG, and the US Air Force Office of Scientific research at TU Berlin and Paderborn University, and has (since 2017) acted as temporary replacement to fill the Full Chair Professorship for macromolecular chemistry and molecular materials at the Institute of Chemistry of the University of Kassel, Germany.

alexander.lorenz@uni-kassel.de

conferenceseries.com

Leonhard Grill, J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-033

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Leonhard Grill

University of Graz, Austria

Manipulation of single molecules at surfaces: switches, wires and motors

Molecular nanotechnology aims to use functional molecules as individual machines or electronic devices. Hence, their self-assembly into pre-defined architectures and the full control over each individual molecule are key objectives. Various examples of functional molecules, ranging from molecular wires to molecular switches and machines that are studied and manipulated at the single-molecule level by scanning tunneling microscopy (STM) under ultrahigh vacuum conditions, will be discussed in this presentation. Molecular wires or molecular nodes with different conjugation pathways can be fabricated from specifically designed molecular building blocks that are connected to two-dimensional networks or one-dimensional chains. In the case of molecular switches, the switching rate can be tuned up and down by only one single atom in the vicinity of the molecule. The same effect is then extended to molecular assemblies where cooperative effects in single molecules are directly observed. The switching process can also be used to trigger a molecular motor where the lateral translation of molecular machines on a surface can be enhanced by light of specific wavelengths that match the absorption properties of the molecule. By comparing molecules with and without a motor unit, the enhanced motion can be directly assigned to the motor that is incorporated in the molecules. STM manipulation gives detailed insight into the physical and chemical processes at the single-molecule level by varying the relevant parameters as tip height over the surface, bias voltage or tunneling current. While the speed is typically of minor importance in these experiments, it becomes crucial when studying so-called nanocars. By implementing a dipole moment into the molecular structure, we could show that very efficient and therefore fast manipulation can be realized. The key property is that no continuous imaging is required, rendering the manipulation fast enough to win the first nanocars race.

Recent Publications:

1. C Nacci et al. (2015) Conductance of a single flexible molecular wire composed of alternating donor and acceptor units. Nature Comm. 6:7397.
2. C Nacci et al. (2016) Covalent assembly and characterization of non-symmetrical single-molecule nodes. Angew. Chem. Int. Ed. 55(44):13724.
3. T Kumagai et al. (2014) Controlling intramolecular hydrogen transfer in a porphycene molecule with single atoms or molecules located nearby. Nature Chem. 6(1):41-46.
4. A Saywell et al. (2016) Light-induced translation of motorized molecules on a surface. ACS Nano. 10(12):10945-10952.
5. G J Simpson et al. (2017) How to build and race a fast nanocar, Nature Nanotech. 12(7):604-606.

Biography

Leonhard Grill is currently a Professor of Physical Chemistry at the University of Graz, Austria, since 2013. He studied physics at the University of Graz and did his PhD thesis at the Laboratorio TASC in Trieste (Italy) in experimental surface physics on electron scattering in ultrathin metal films (group of Silvio Modesti). He is an experimental physicist specialized in the study of single functional molecules. By using scanning probe microscopy, his group is able to image and manipulate individual atoms and molecules adsorbed at surfaces and to characterize specific molecular functions. In this way electronic, electrical, optical or mechanical properties of individual molecules are controlled with the goal to obtain fundamental physical and chemical understanding of these processes. He received the Feynman Prize in Nanotechnology (2011).

leonhard.grill@uni-graz.at